



HAL
open science

Calculation appendix to the paper "N₂ exchanges in hyperbaric environments: towards a model based on physiological gas transport (O₂ and CO₂) "

Michael Theron, Alexis Blasselle

► To cite this version:

Michael Theron, Alexis Blasselle. Calculation appendix to the paper "N₂ exchanges in hyperbaric environments: towards a model based on physiological gas transport (O₂ and CO₂) ". 2024. hal-04722226

HAL Id: hal-04722226

<https://hal.science/hal-04722226v1>

Submitted on 9 Oct 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution - NonCommercial - NoDerivatives 4.0 International License

Calculation appendix

Gas exchanges in hyperbaric environments: towards a physiological model

Alexis Blasselle, Michael theron

This appendix serves various purposes : it gives the required mathematical tools needed for the computations made in the corpus of the article, it demonstrates the existence of solutions to the differential systems presented in the article and it presents the results of another implementation of a numerical solution of those systems.

1 Study of the function f

In this section, some basic properties of the function f defined in the article are given. The function H is defined over \mathbb{R} by $H(x) = \frac{1}{x^3 + bx}$ and satisfies $\lim_{x \rightarrow +\infty} H(x) = 0$. 1. By denoting $\lambda = O_{xc}Hb$ and $\alpha = \alpha_{O_2}$, f can be written :

$$f(x) = \lambda H(x) + \alpha x$$

H and f are differentiable over \mathbb{R}

$$\begin{aligned} H'(x) &= \frac{(3x^2 + b)(x^3 + bx + a) - (3x^2 + b)(x^3 + bx)}{(x^3 + bx + a)^2} \\ &= \frac{a(3x^2 + b)}{(x^3 + bx + a)^2} \end{aligned}$$

so

$$f'(x) = \frac{a \lambda (3x^2 + b)}{(x^3 + bx + a)^2} + \alpha \quad (1)$$

and from this definition, the following property can be written :

Property 1 f' is continuous, differentiable and bounded over \mathbb{R} and satisfies

$$f'(x) \xrightarrow{x \rightarrow +\infty} \alpha \quad \text{and} \quad f'(x) \xrightarrow{x \rightarrow -\infty} \alpha$$

Please note also that, as $a > 0$, $\alpha > 0$ and $\lambda > 0$, we have that

$$\forall x \in \mathbb{R}, \quad f'(x) > 0 \quad (2)$$

2 Notations and hypothesis

2.1 Notations and derivatives

The following notations are adopted, to simplify the equations

◇ 1 : inspired air

- ◇ 2 : airways
- ◇ 3 : alveolar gas
- ◇ 4 : alveolar blood
- ◇ 5 : arterial blood
- ◇ 6 : capillary blood
- ◇ 7 : venous blood
- ◇ 8 : tissue

Besides, the following vector is defined :

$$\forall t \in \mathbb{R} \quad X(t) = (P_2(t), \dots, P_8(t))^T$$

When the perfect gas law is satisfied, one can write $P_i V_i = Q_i R T$. Hence

$$\frac{dQ_i}{dt} = \frac{1}{RT} V_i \frac{dP_i}{dt} + \frac{1}{RT} P_i \frac{dV_i}{dt}$$

When $C_i = f(P_i)$, as $Q_i = V_i C_i$ for $i = 4, \dots, 8$, Q_i time derivative can be expressed as follows :

$$\frac{dQ_i}{dt} = V_i \frac{dP_i}{dt} f'(P_i) + f(P_i) \frac{dV_i}{dt}$$

2.2 Hypothesis

The following hypothesis are made on the input parameters. P_1 is given by, with M the considered gas

$$P_1(t) = f_r(M)(AP(t) - P_{H_2O})$$

Hypothesis 1 *The function AP is differentiable over \mathbb{R} and its derivative is continuous over \mathbb{R} . Hence, the property is also true for P_1 , so $P_1 \in C^1(\mathbb{R})$. AP is a known input parameter.*

Hypothesis 2 *The volumes and their derivatives are continuous over \mathbb{R} , so $\forall i = 1, \dots, 7$, $V_i \in C^1(\mathbb{R})$. They are known input parameters.*

3 Oxygen differential system

3.1 General case

The assumption 2 holds. In the following equations, K_i , α_i , \dot{Q} and $\dot{M}O_2$ are known constants defined in the article.

$$\begin{aligned}\frac{dP_2}{dt} &= \frac{\dot{V}}{V_2}P_1 - \frac{P_2}{V_2} \left(\frac{dV_2}{dt} + \dot{V} + K_1RT \right) + \frac{K_1RT}{V_2}P_3 \\ \frac{dP_3}{dt} &= -\frac{P_3}{V_3} \left[\frac{dV_3}{dt} + RT(K_1 + K_2) \right] + \frac{RT}{V_3} [K_1P_2 + K_2P_4] \\ \frac{dP_4}{dt} &= \frac{1}{V_4 f'(P_4)} \left[-f(P_4) \frac{dV_4}{dt} + K_2(P_3 - P_4) + \dot{Q}(f(P_7) - f(P_4)) \right] \\ \frac{dP_5}{dt} &= \frac{1}{V_5 f'(P_5)} \left[-f(P_5) \frac{dV_5}{dt} + \dot{Q}(f(P_4) - f(P_5)) \right] \\ \frac{dP_6}{dt} &= \frac{1}{V_6 f'(P_6)} \left[-f(P_6) \frac{dV_6}{dt} + \dot{Q}(f(P_5) - f(P_6)) - K_3(P_6 - P_8) \right] \\ \frac{dP_7}{dt} &= \frac{1}{V_7 f'(P_7)} \left[-f(P_7) \frac{dV_7}{dt} + \dot{Q}(f(P_6) - f(P_7)) \right] \\ \frac{dP_8}{dt} &= \frac{1}{\alpha_8 V_8} \left[-\alpha_8 P_8 \frac{dV_8}{dt} + K_3(P_6 - P_8) - \dot{M}O_2 \right]\end{aligned}$$

The previous system, well defined thanks to (2) can be written under the form

$$\dot{X} = F(t, X) \tag{3}$$

F belonging to $\mathcal{C}^1(\mathbb{R} \times \mathbb{R}^7; \mathbb{R}^7)$, the Cauchy-Lipschitz theorem can be applied to this system, leading to the following theorem :

Theorem 1 *Under the assumptions 1 and 2, for every $t_0 \in \mathbb{R}$ and for every $X_0 \in \mathbb{R}^7$, the system (3) has a unique solution satisfying $X(t_0) = X_0$.*

Remark 1 *Please note that the source term is actually coming from $P_1(t)$*

3.2 Steady volumes

The assumption of steady volumes is made, leading to

$$\frac{dV_i}{dt} = 0$$

and one obtains the following simplified system :

$$\begin{aligned}\frac{dP_2}{dt} &= \frac{\dot{V}}{V_2}P_1 - \frac{\dot{V} + K_1RT}{V_2}P_2 + \frac{K_1RT}{V_2}P_3 \\ \frac{dP_3}{dt} &= -\frac{RT}{V_3}(K_1 + K_2)P_3 + \frac{RT}{V_3}[K_1P_2 + K_2P_4] \\ \frac{dP_4}{dt} &= \frac{1}{V_4f'(P_4)} \left[K_2(P_3 - P_4) + \dot{Q}(f(P_7) - f(P_4)) \right] \\ \frac{dP_5}{dt} &= \frac{\dot{Q}}{V_5f'(P_5)} [f(P_4) - f(P_5)] \\ \frac{dP_6}{dt} &= \frac{1}{V_6f'(P_6)} \left[\dot{Q}(f(P_5) - f(P_6)) - K_3(P_6 - P_8) \right] \\ \frac{dP_7}{dt} &= \frac{\dot{Q}}{V_7f'(P_7)} [f(P_6) - f(P_7)] \\ \frac{dP_8}{dt} &= \frac{1}{\alpha_8V_8} \left[K_3(P_6 - P_8) - \dot{M}O_2 \right]\end{aligned}$$

The theorem 1 holds for this particular case, and implies existence and uniqueness of a solution to this system for a given initial value.

3.3 Numerical implementation

The system defined in 3.2 has been implemented in Scilab, separately and independently from the implementation that produced the figures presented in the article, in order to check the values and to verify that no mistake has been made. The implementation was made by a different co-author. The 2 codes lead to the same numerical results, and the Scilab representations are given below :

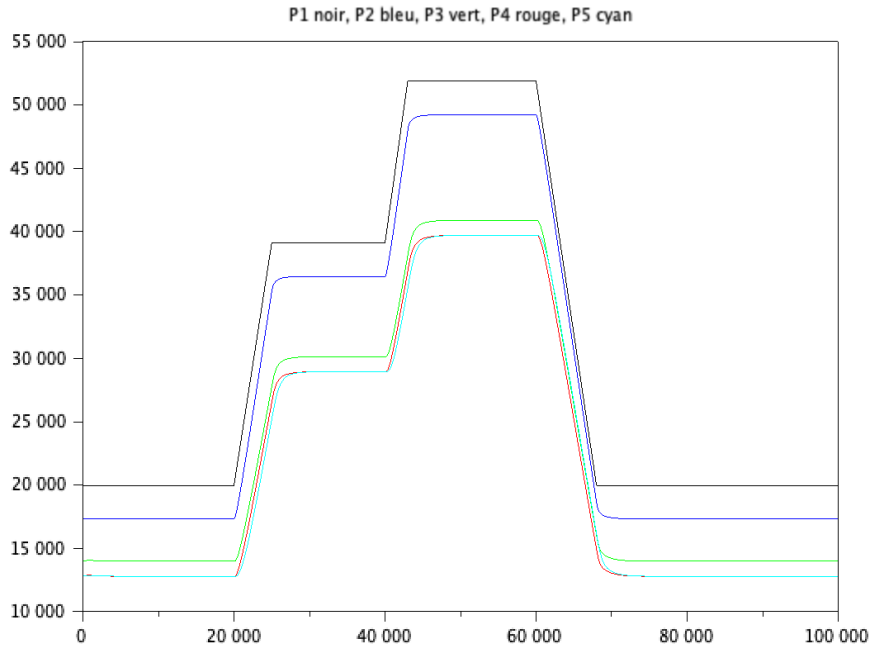


FIGURE 1 – Pressures P_1 to P_5 included

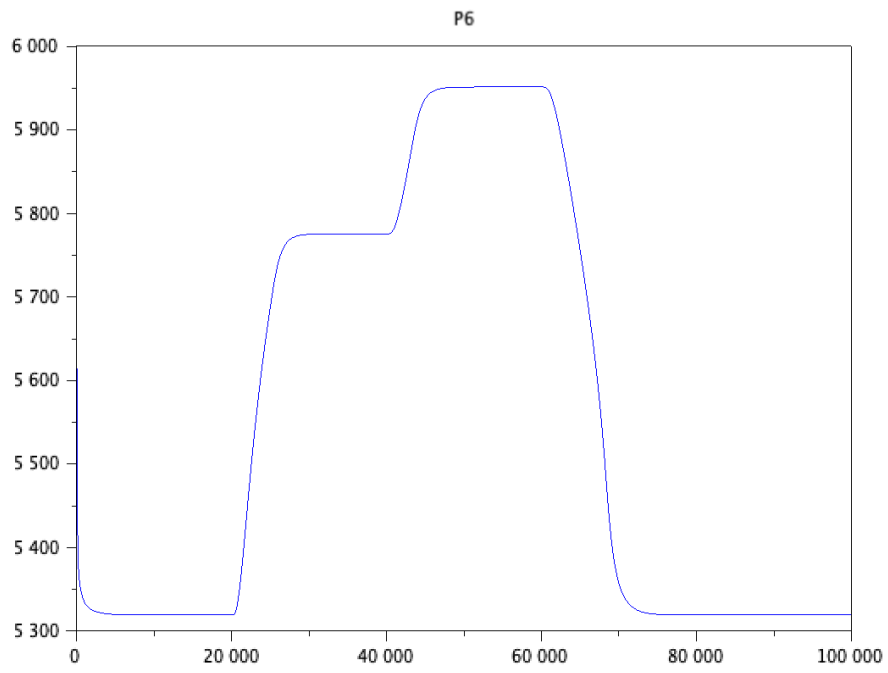


FIGURE 2 – Pressure *P6*

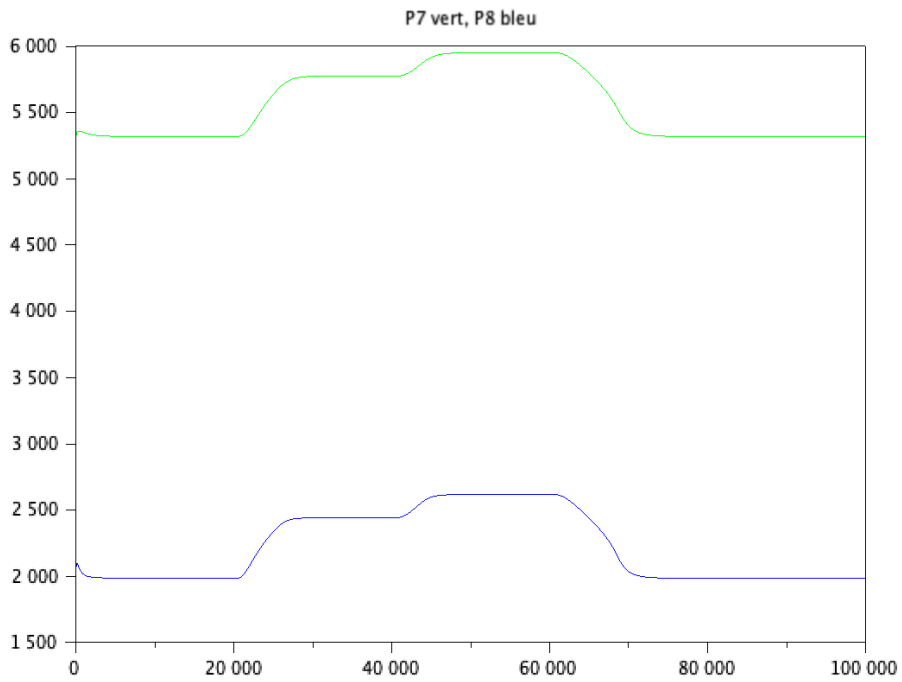


FIGURE 3 – Pressures *P7* and *P8*

4 Nitrogen differential case

4.1 General case

The assumption is made that the time derivatives of the volumes are known, and that the equations for nitrogen can be derived from the oxygen ones

$$\begin{aligned}
 \frac{dP_2}{dt} &= \frac{\dot{V}}{V_2} P_1 - \frac{P_2}{V_2} \left(\frac{dV_2}{dt} + \dot{V} + K_1 RT \right) + \frac{K_1 RT}{V_2} P_3 \\
 \frac{dP_3}{dt} &= -\frac{P_3}{V_3} \left[\frac{dV_3}{dt} + RT(K_1 + K_2) \right] + \frac{RT}{V_3} [K_1 P_2 + K_2 P_4] \\
 \frac{dP_4}{dt} &= \frac{1}{V_4 \alpha_{N_2}} \left[-\alpha_{N_2} P_4 \frac{dV_4}{dt} + K_2 (P_3 - P_4) + \dot{Q} \alpha_{N_2} (P_7 - P_4) \right] \\
 \frac{dP_5}{dt} &= \frac{\dot{Q}}{V_5} \left[-\alpha_{N_2} P_5 \frac{dV_5}{dt} + P_4 - P_5 \right] \\
 \frac{dP_6}{dt} &= \frac{1}{V_6 \alpha_{N_2}} \left[-\alpha_{N_2} P_6 \frac{dV_6}{dt} + \dot{Q} \alpha_{N_2} (P_5 - P_6) - K_3 (P_6 - P_8) \right] \\
 \frac{dP_7}{dt} &= \frac{\dot{Q}}{V_7} \left[-\alpha_{N_2} P_7 \frac{dV_7}{dt} + P_6 - P_7 \right] \\
 \frac{dP_8}{dt} &= \frac{1}{\alpha_8 V_8} \left[-\alpha_8 P_8 \frac{dV_8}{dt} + K_3 (P_6 - P_8) \right]
 \end{aligned}$$

This system is exactly similar to the system (3) and by the same type of proof, one gets existence and uniqueness of a solution.

4.2 Steady volumes

If the volumes are constant over time, the system for the nitrogen writes

$$\begin{aligned}
 \frac{dP_2}{dt} &= \frac{\dot{V}}{V_2} P_1 - \frac{\dot{V} + K_1 RT}{V_2} P_2 + \frac{K_1 RT}{V_2} P_3 \\
 \frac{dP_3}{dt} &= -\frac{RT}{V_3} (K_1 + K_2) P_3 + \frac{RT}{V_3} [K_1 P_2 + K_2 P_4] \\
 \frac{dP_4}{dt} &= \frac{1}{\alpha_N V_4} \left[K_2 P_3 - P_4 (K_2 + \alpha_N \dot{Q}) + \alpha_N \dot{Q} P_7 \right] \\
 \frac{dP_5}{dt} &= \frac{\dot{Q}}{V_5} [P_4 - P_5] \\
 \frac{dP_6}{dt} &= \frac{1}{\alpha_N V_6} \left[\alpha_N \dot{Q} P_5 - P_6 (\alpha_N \dot{Q} + K_3) + K_3 P_8 \right] \\
 \frac{dP_7}{dt} &= \frac{\dot{Q}}{V_7} [P_6 - P_7] \\
 \frac{dP_8}{dt} &= \frac{K_3}{\alpha_8 V_8} [P_6 - P_8]
 \end{aligned}$$

This system is linear and can be simply written

$$\dot{X}(t) = AX(t) + U(t) \quad A \in \mathcal{M}_7(\mathbb{R}) \quad (4)$$

with

$$U(t) = \left(\frac{\dot{V}}{V_2} P_1(t), 0, 0, 0, 0, 0, 0 \right)^T \quad (5)$$

Theorem 2 For every vector $X_0 \in \mathbb{R}^7$ and for every $t_0 \in \mathbb{R}$ the system (4), with (5) has a unique solution satisfying $X(t_0) = X_0$, which is

$$X(t) = \exp(tA) \left[X_0 + \int_0^t \exp(-sA)U(s) ds \right]$$

Proof : One has to consider the equation with no right hand side, $\dot{Z} = AZ$, whose solution is $Z(t) = \exp(tA)Z(0)$, and then use a varying constant method, writing $X(t) = \exp(tA)\Lambda(t)$, and derive this expression to find the explicit expression of Λ . \square

Remark 2 Even if this elegant exact solution was found, it would require the diagonalization of the matrix A in order to be properly implemented. Hence, a Runge-Kutta 4 method was preferred, and implemented by 2 different persons, with no exchanges apart from the sharing of the input data, and the final comparison.

4.3 Numerical implementation of the N_2 model

The N_2 model with steady volumes described in the previous paragraph has been implemented by 2 different persons with a Runge-Kutta 4 method, and the 2 codes converge towards values that are very similar. The table 4 shows the initial values and the table values obtained after a 100-minute simulation. In order to see the stability of the 2 codes even with drastic changes, the assumption was made that all the compartments were free of N_2 at the initial time. The table 5 shows the comparison between the 2 codes : *Computed* corresponds to an Excel computation, while *Implemented* refers to a VBA code. One can see that the 2 different codes are very close one from another.

| Grandeur | Value | Unit |
|--------------------------------------|------------|-------------|
| Diverses | | |
| Qp | 4.200 | L/min |
| Vp | 8.100 | L/min |
| alpha_N | 0.00000602 | |
| alpha_8 | 0.00001064 | mmol/min/kg |
| Compartment volumes | | |
| V2 | 1.5 | L |
| V3 | 1.0 | L |
| V4 | 0.5 | L |
| V5 | 1.7 | L |
| V6 | 0.5 | L |
| V7 | 3.0 | L |
| V8 | 70.0 | L |
| Initial pressures | | |
| P10 | 75 074.00 | Pa |
| P20 | 0.00 | Pa |
| P30 | 0.00 | Pa |
| P40 | 0.00 | Pa |
| P50 | 0.00 | Pa |
| P60 | 0.00 | Pa |
| P70 | 0.00 | Pa |
| P80 | 0.00 | Pa |
| Diffusion coefficients | | |
| K1 | 0.00267 | mmol/min/Pa |
| K2 | 0.00748 | mmol/min/Pa |
| K3 | 0.00267 | mmol/min/Pa |
| Temperature and perfect gas constant | | |
| Tpt | 310.150 | K |
| R | 8.314 | kPa·L/mol/K |

FIGURE 4 – Initial values for the computation

And 6 is a caption of the evolution of the different N_2 pressures in all the different compartments.

| Comparison between the 2 codes, T = 100 minutes | | | |
|---|-----------|-------------|------------|
| Pressure | Computed | Implemented | Error in % |
| P2 | 75 050.81 | 75 050.35 | 0.0006 |
| P3 | 75 023.28 | 75 022.73 | 0.0007 |
| P4 | 75 013.54 | 75 012.95 | 0.0008 |
| P5 | 75 012.72 | 75 012.13 | 0.0008 |
| P6 | 72 199.40 | 72 189.00 | 0.0144 |
| P7 | 72 130.40 | 72 119.84 | 0.0146 |
| P8 | 72 172.88 | 72 162.39 | 0.0145 |

FIGURE 5 – Comparison between the 2 codes

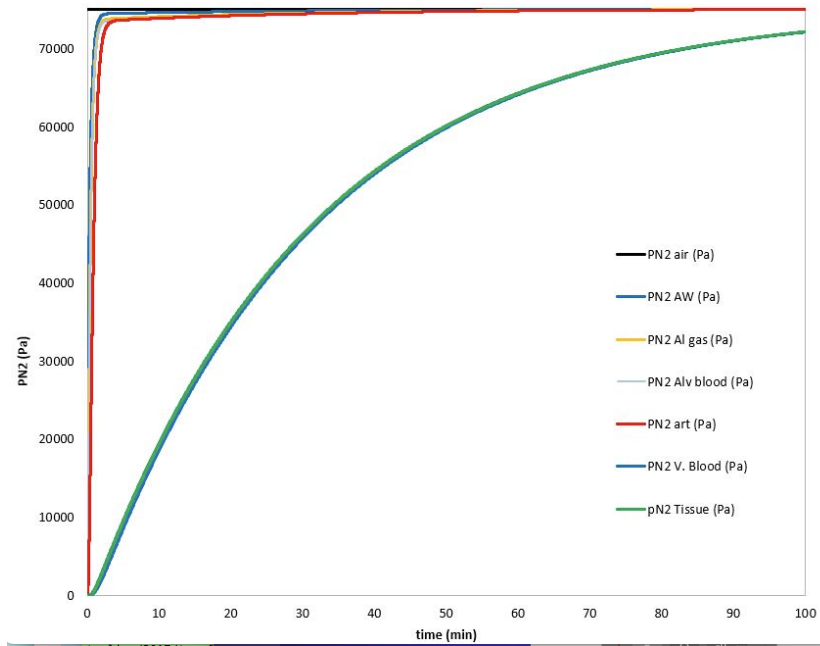


FIGURE 6 – Evolution of the different N_2 pressures in all the compartments

5 Various functions for the CO_2 model

In this part, we describe several functions needed for the CO_2 model. As some of them appear in the denominators of the equations, we have to show that they do not vanish. As we could not succeed to show it theoretically, we checked their numerical values.

5.1 g function

Notations In the article, the carbon dioxide pressure relates to the pH through the following function

$$P(CO_2) = g(pH) = \frac{1}{\alpha_{CO_2}} (a pH + b) 10^{pK - pH}$$

Please note that the coefficient a and b used there are not the ones used previously. We use the following notation for the study of g :

$$\lambda = \frac{10^{pK}}{\alpha_{CO_2}}$$

which then writes

$$g(x) = \lambda(ax + b) 10^{-x}$$

Please note the following assumption

Hypothesis 3 The coefficient a satisfies $a < 0$.

Study of g As we need to find the pH as a function of the carbon dioxide pressure, we have seen if g is a bijection, and for this to study it.

$$g'(x) = \lambda [a - (ax + b) \ln(10)] 10^{-x}$$

which vanishes on

$$x_0 = \frac{1}{\ln(10)} - \frac{b}{a} \quad (6)$$

and we have that

$$\begin{aligned} g(x) &\underset{x \rightarrow -\infty}{\rightarrow} +\infty & \text{and} & & g(x) &\underset{x \rightarrow +\infty}{\rightarrow} 0^- \\ g'(x) &\underset{x \rightarrow -\infty}{\rightarrow} -\infty & \text{and} & & g'(x) &\underset{x \rightarrow +\infty}{\rightarrow} 0^+ \end{aligned}$$

and from this we get that g is strictly decreasing on $] -\infty; x_0]$ and strictly increasing on $[x_0; +\infty[$. Hence, it is a bijection on each of those intervals, but we will have to make sure that we look for its reverse function on **one or the other intervals**. We note $h = g^{-1}$ in what follows. Here is a graphical representation of g on a reduced interval

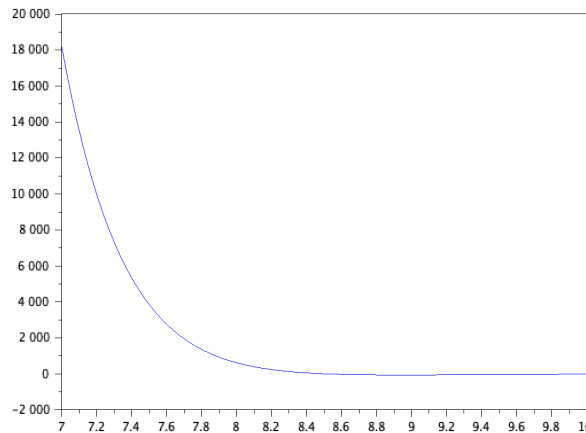


FIGURE 7 – Function g on a reduced interval

Numerical application An explicit and general expression of the reverse function of g cannot be found as it uses the Lambert function, but some softwares can provide approximate values. With the following values

$$a = -21.6 \quad b = 183.84 \quad \alpha_{CO_2} = 2.2502 \cdot 10^{-4} \quad pK = 6.1 \quad (7)$$

one gets x_0

$$x_0 \approx 8.94$$

This is a very high value for the blood pH , hence one can reverse g on $] -\infty; x_0]$, and with a software for approaching h , we get an approximate function \hat{h} defined by

$$\hat{h}(x) = c_0 + c_1 \ln x + c_2 (\ln x)^2 + c_3 (\ln x)^3 + c_4 (\ln x)^4 \quad (8)$$

As the pH can only be positive, we can decide to study and define g only on a smaller interval. But similarly, as the CO_2 pressure is supposed to be positive, we can restrict again the interval and study g only where she is positive. Finding the value for which g vanishes gives :

$$g(\tilde{x}) = 0 \quad \Longleftrightarrow \quad \tilde{x} = \frac{-b}{a} \approx 8.51$$

and note that $\tilde{x} < x_0$ by construction.

Definition of h We decide to study and reverse g on the interval $I = [0; \tilde{x}]$. The reverse function h of g is defined on $J = g(I) = [0; g(0)]$ with $g(0) = \lambda b > 0$. From this we get the following definitions for the intervals

$$I = \left[0; \frac{-b}{a}\right] \quad \text{and} \quad J = [0; \lambda b] \quad (9)$$

Numerical application gives that $g(0) \approx 1.029 \cdot 10^{12}$.

Derivative of the reverse h Even if we found an approximative function close enough from h , nothing guarantees that its derivative will be close from h' . Hence, it appears safer to use a simple trick, by deriving the relation $g(h(x)) = x$

$$h'(x) g'(h(x)) = 1$$

one gets

$$h'(x) = \frac{10^{h(x)}}{\lambda [a - (ah(x) + b) \ln(10)]} \quad (10)$$

As we do not have the explicit expression of h , we will use \hat{h} in (10) but it will be less risky than deriving (8), as we do not know the closeness between \hat{h}' and h' . From the definition of h , please note that one can use

$$\forall x \in J, \quad 0 < h(x) < \frac{-b}{a}$$

to establish the following inequality for its derivative

$$\frac{10^{h(x)}}{\lambda a} < h'(x) < \frac{10^{h(x)}}{\lambda(a - b \ln 10)} < 0 \quad (11)$$

5.2 R function

This function is defined on J by

$$R(x) = \alpha_{\text{CO}_2} x (1 + 10^{h(x) - pK}) \quad (12)$$

as a composition of \mathcal{C}^1 function on the intervals on which they are defined, R is of class \mathcal{C}^1 .

$$\frac{R'(x)}{\alpha_{\text{CO}_2}} = 1 + [1 + x h'(x) \ln(10)] 10^{h(x) - pK} \quad (13)$$

So far, even if we established the inequality (11), we did not succeed in proving that R' will not vanish on the considered interval, so we decided to study its values on a pressure interval relevant for our study, namely considering a minimum pressure of 4,000 and a maximum pressure of 15,000.

As one can see, even if R' does not vanish, its values are quite small, indicating that the system may present some numerical instabilities.

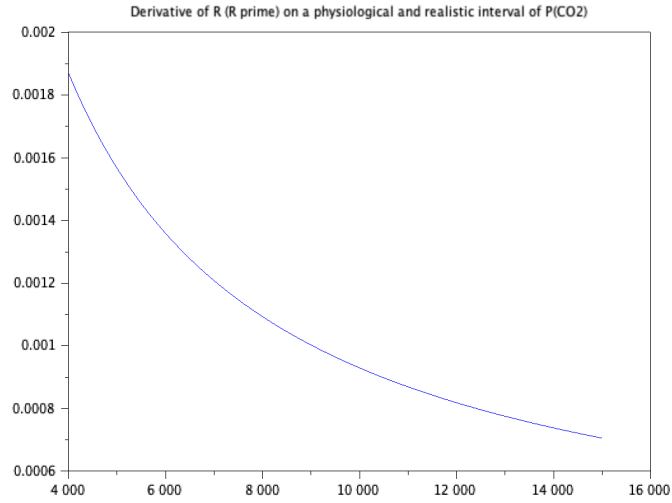


FIGURE 8 – R' on a relevant pressure interval

5.3 M function

This function is defined by

$$M(x) = R(x) \left[1 + \frac{0.0289[Hb]}{(3.352 - 0.456 Sat)(h(x) - 8.142)} \right]$$

The terms on the lower part of the fraction cannot vanish, as the pH blood can never reach a value as high as 8.142 and as the saturation Sat is comprised between 0 and 1. We note

$$\zeta = 8.142 \quad \text{and} \quad \mu = \frac{0.0289[Hb]}{(3.352 - 0.456 Sat)} \quad (14)$$

which enables to write

$$M(x) = R(x) \left[1 + \frac{\mu}{h(x) - \zeta} \right] \quad (15)$$

As for R , M can be derived on the proper interval, and one gets

$$M'(x) = R'(x) \left[1 + \frac{\mu}{h(x) - \zeta} \right] - \mu R(x) \frac{h'(x)}{(h(x) - \zeta)^2} \quad (16)$$

Now, for what follows, we need to see if M' can vanish or not. The values for Hb and Sat are the following

$$Hb = 2.19117647058824 \text{ mmol/L} \quad \text{and} \quad Sat = 0.99$$

We proceed as for R' and study the numerical values of M' , whose values are very close from the R' 's ones.

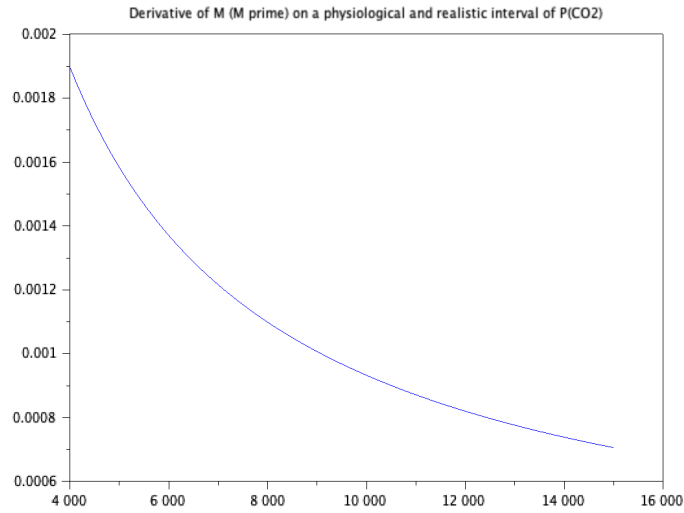


FIGURE 9 – M' on a relevant pressure interval

6 Carbon dioxide model

6.1 Equations

The assumption 2 still holds, leading to the following system for the carbon dioxide CO_2

$$\begin{aligned} \frac{dP_2}{dt} &= \frac{\dot{V}}{V_2} P_1 - \frac{\dot{V} + K_1 RT}{V_2} P_2 + \frac{K_1 RT}{V_2} P_3 \\ \frac{dP_3}{dt} &= -\frac{RT}{V_3} (K_1 + K_2) P_3 + \frac{RT}{V_3} [K_1 P_2 + K_2 P_4] \\ \frac{dP_4}{dt} &= \frac{1}{V_4 M'(P_4)} \left[K_2 (P_3 - P_4) + \dot{Q} (M(P_7) - M(P_4)) \right] \\ \frac{dP_5}{dt} &= \frac{\dot{Q}}{V_5 M'(P_5)} [M(P_4) - M(P_5)] \\ \frac{dP_6}{dt} &= \frac{1}{V_6 M'(P_6)} \left[\dot{Q} (M(P_5) - M(P_6)) - K_3 (P_6 - P_8) \right] \\ \frac{dP_7}{dt} &= \frac{\dot{Q}}{V_7 M'(P_7)} [M(P_6) - M(P_7)] \\ \frac{dP_8}{dt} &= \frac{1}{V_8 R'(P_8)} \left[K_3 (P_6 - P_8) + RQ \dot{M}O_2 \right] \end{aligned}$$

Remark 3 Be careful, RQ is a variable itself, and has no link whatsoever with the constant R .

6.2 Steady state

If one considers an input pressure P_1 constant over time, the system is supposed to stabilize for an infinite time towards a limit steady state. This state would be characterized by null time derivatives, leading to the following set of equations, in which **we keep for the moment the same notations than before**

$$\dot{V}P_1 - (\dot{V} + K_1RT)P_2 + K_1RTP_3 = 0 \quad (17)$$

$$-RT(K_1 + K_2)P_3 + RT[K_1P_2 + K_2P_4] = 0 \quad (18)$$

$$K_2(P_3 - P_4) + \dot{Q}(M(P_7) - M(P_4)) = 0 \quad (19)$$

$$M(P_4) - M(P_5) = 0 \quad (20)$$

$$\dot{Q}(M(P_5) - M(P_6)) - K_3(P_6 - P_8) = 0 \quad (21)$$

$$M(P_6) - M(P_7) = 0 \quad (22)$$

$$K_3(P_6 - P_8) + RQ\dot{M}O_2 = 0 \quad (23)$$

Considering the previous sign study that we made of M' , we know that M is a bijection on the interval of interest, hence (22) and (20) lead to

$$P_4 = P_5 \quad \text{and} \quad P_6 = P_7$$

combining now (21) and (23) one gets

$$\dot{Q}(M(P_4) - M(P_7)) = -RQ\dot{M}O_2$$

and combining this with (19), one gets

$$K_2(P_3 - P_4) = -RQ\dot{M}O_2$$

and introducing this in (18)

$$K_1(P_2 - P_3) = -RQ\dot{M}O_2$$

and then back to (17)

$$P_2 = P_1 + \frac{RT}{\dot{V}} RQ\dot{M}O_2$$

which can be used in all the other equations to find the other limit steady state values for the other pressures. One can then finally write

$$P_2 = P_1 + \frac{RT}{\dot{V}} RQ\dot{M}O_2$$

$$P_3 = P_2 + \frac{RQ\dot{M}O_2}{K_1}$$

$$P_4 = P_3 + \frac{RQ\dot{M}O_2}{K_2}$$

$$P_5 = P_4$$

$$P_6 = P_7$$

$$M(P_7) = M(P_4) + \frac{RQ\dot{M}O_2}{\dot{Q}}$$

$$P_8 = P_6 + \frac{RQ\dot{M}O_2}{K_3}$$

6.3 Numerical implementation

The system has been implemented with 2 different numerical methods, and, with no exterior variations, the 2 models converge towards values that are approximately the ones obtained from the steady state. The following table 10 shows how the 2 codes reach the same value what can be computed from the steady state. The column titled *computed value* corresponds to an implementation with Excel, while the column titled *Implemented value* gives the value obtained with a VBA code.

| Data | Computed value | Implemented value | Unit |
|--------------------------------------|-------------------|-------------------|-------------|
| Miscellaneous constants | | | |
| Qp | 4.200 | 4.200 | L/min |
| Vp | 8.100 | 8.100 | L/min |
| RRQQ | 0.700 | 0.700 | |
| MpO2 | 8.333 | 8.333 | mmol/min/kg |
| Temperature and Perfect gas constant | | | |
| Tpt | 310.150 | 310.150 | K |
| R | 8.314 | 8.314 | kPa·L/mol/K |
| Diffusion coefficients | | | |
| K1 | 0.002132007163556 | 0.002 | mmol/min/Pa |
| K2 | 0.005970 | 0.006 | mmol/min/Pa |
| K3 | 0.002132007163556 | 0.002 | mmol/min/Pa |
| Steady state pressures | | | |
| P1 | 38.03 | 38.03 | Pa |
| P2 | 1 895.1 | 1 884.0 | Pa |
| P3 | 4 631.0 | 4 604.0 | Pa |
| P4 | 5 608.2 | 5 575.0 | Pa |
| P5 | 5 608.2 | 5 575.0 | Pa |
| P6 | 6 593.0 | 6 593.0 | Pa |
| P7 | 6 593.0 | 6 593.0 | Pa |
| P8 | 9 329.0 | 9 316.0 | Pa |
| Verification for M(P7) | | | |
| h(P4) | 7.385 | 7.387 | pH unit |
| R(P4) | 25.586 | 25.539 | mmol/L |
| grosse parenthèse (P4) | 0.987 | 0.987 | pH unit |
| M(P4) | 25.253 | 25.205 | mmol/L |
| M(P4)+RRQQ*MpO2/Qp | 26.642 | 26.594 | mmol/L |
| h(P7) | 7.334 | 7.334 | pH unit |
| R(P7) | 26.910 | 26.910 | mmol/L |
| grosse parenthèse (P7) | 0.988 | 0.988 | pH unit |
| M(P7) | 26.581 | 26.581 | mmol/L |

FIGURE 10 – Convergence towards the steady state